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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 12:53:52 ON 15 APR 2008

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 12:54:11 ON 15 APR 2008

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2008 HIGHEST RN 1014671-54-5

DICTIONARY FILE UPDATES: 14 APR 2008 HIGHEST RN 1014671-54-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

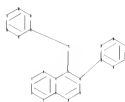
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10-598,246.str



```

chain nodes :
23
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22
chain bonds :
7-23  8-12  22-23
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  11-12  11-16  12-13  13-14
14-15  15-16  17-18  17-22  18-19  19-20  20-21  21-22
exact/norm bonds :
7-23  22-23
exact bonds :
8-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  11-12  11-16  12-13  13-14
14-15  15-16  17-18  17-22  18-19  19-20  20-21  21-22
isolated ring systems :
containing 1 : 11 : 17 :
```

G1:O,S

Match level :

04/17/2008

10-598,246.trn

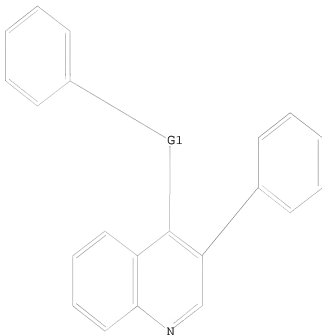
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 12:55:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 9 TO 360

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

04/17/2008

10-598,246.trn

=> s l1 sss full

FULL SEARCH INITIATED 12:55:33 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 122 TO ITERATE

100.0% PROCESSED 122 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

L3

25 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

179.28

179.49

FILE 'CAPLUS' ENTERED AT 12:55:41 ON 15 APR 2008

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FILE COVERS 1907 - 15 Apr 2008 VOL 148 ISS 16

FILE LAST UPDATED: 14 Apr 2008 (20080414/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4

5 L3

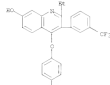
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YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

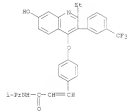


RI 828300-13-6 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

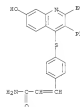


RI 828300-14-7 CAPLUS
 CH 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 863713-19-6 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]- (CA INDEX NAME)



IT 863713-19-7
 RI: RCT (Reactant); RACT (Reactant or reagent)
 Preparation of substituted quinoline compounds. For use as selective
 estrogen receptor modulator to treat various diseases)
 RI 863713-19-7 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 863713-16-4 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



RI 863713-17-5 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

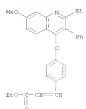


IT 828300-18-1F, 2-Ethyl-3-phenyl-4-(4-bromophenoxy)-7-methoxyquinoline 828300-52-7P
 RI: RCT (Reactant); RACT (Reactant or reagent); PREP (Preparation); RACT (Reactant or reagent)
 Preparation of substituted quinoline compounds. For use as selective
 estrogen receptor modulator to treat various diseases)
 RI 828300-18-3 CAPLUS
 CH Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



RI 828300-22-7 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

14 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

ACCESSION NUMBER: 20041307077 CAPLUS
 DOCUMENT NUMBER: 14212060
 TITLE: Discovery of Novel Quinoline-Based Estrogen Receptor Ligands Using Peptide Interaction Profiling
 AUTHOR(S): Beckwith, William J.; Patel, Ravi S.; Liang, Xi; Hlane, Jean-Sébastien E.; Meyer, Dennis O.; Willson, Timothy W.; Johnson, Marie A.; Hubbell, Dan W.; Miller, Lisa A.; Pearson, Kenneth R.; Sunwoo, Catherine A.; Shear, Jean
 CORPORATE SOURCE: GlaxoSmithKline Research Development, Research Triangle Park, NC, 27709-2739, USA
 SOURCE: Journal of Medicinal Chemistry (2005), 48(6), 2243-2247
 CUBRID: CUBRID; ISSN: 0022-2625
 PUBLISHED: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 14212060
 AB Traditional approaches to discovery of selective estrogen receptor modulators (SERMs) have relied on ER binding and cell-based estrogen response element-driven assays to identify compounds that act orthoprotective but nonproliferative in breast and uterine tissues. To discover new classes of potential SERMs, we have employed a cell-free microsphere-based binding assay to rapidly characterize ERα interactions with conformation-changing molecules or phage display peptide libraries.
 Peptide profiles of constrained triazoles were compared to known proliferative and nonproliferative ERα ligands to discover potent quinoline-based ligands with minimal Ishikawa cell stimulation.

IT

828300-01-81 828300-08-9 828300-09-0
 828300-10-39 828300-11-49 828300-12-59
 828300-13-49 828300-14-79 828300-15-59
 ERα PAC (Pharmacological activity); ERα (Synthetic preparation); ERα (Therapeutic use); ERα (Biological study); ERα (Preparation); ERα (Use)

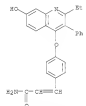
(6) discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)

ER 828300-01-8 CAPLUS
 ER 828300-08-9 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-4-quinolinyl]oxy[phenyl]- (CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

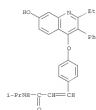


ER 828300-09-3 CAPLUS
 ER 828300-09-3 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-4-quinolinyl]oxy[phenyl]- (CA INDEX NAME)

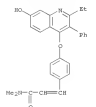


ER 828300-09-0 CAPLUS
 ER 828300-09-0 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N-(1-methylhexyl)- (CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

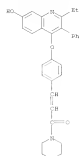


ER 828300-10-3 CAPLUS
 ER 828300-10-3 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N-(1-methylhexyl)- (CA INDEX NAME)



ER 828300-11-4 CAPLUS
 ER 828300-11-4 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-1-oxo-2-propenyl]- (SCI) (CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 828700-12-5 CAPLUS
CN 2-Propenoic acid,
3-[4-[(1-ethoxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]-
(CA INDEX NAME)



HN 828700-13-6 CAPLUS
CN 2-Propenoic acid,
3-[4-[(1-ethyl-7-hydroxy-3-[(trifluoromethyl)phenyl]-4-quinolinyl)oxy]phenyl]-
(CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



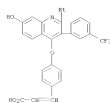
IT 828700-18-1P 828700-18-1P 828700-20-5P
828700-21-6P 828700-22-7P 828700-23-8P
828700-24-9P 828700-25-0P
XL NCT (Neatant); SPH (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(Discovery of novel quinoline-based estrogen receptor ligands using
peptide interaction profiling)

HN 828700-19-1 CAPLUS
CN Quinoline, 4-[(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl]- (CA INDEX
NAME)



HN 828700-19-2 CAPLUS
CN Quinoline, 4-[(4-bromophenoxy)-7-methoxy-2,3-diphenyl]- (CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 828700-14-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl)-4-quinolinyl]oxy]phenyl]-
(CA INDEX NAME)

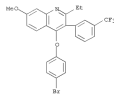


HN 828700-15-8 CAPLUS
CN 7-Quinolone, 4-[(4-[(2-(dimethylamino)ethoxy]phenoxy)-2-ethyl-3-phenyl]-
(CA INDEX NAME)

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 828700-20-5 CAPLUS
CN Quinoline, 4-[(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl]-
(trifluoromethyl)phenyl]- (CA INDEX NAME)



HN 828700-21-6 CAPLUS
CN Quinoline, 4-[(3-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl]- (CA INDEX
NAME)

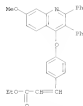


HN 828700-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl)-4-quinolinyl]oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)

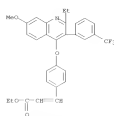


20 828360-23-9 CAPLOS
 CN 2-Propenoic acid,
 3-[4-[(1-methoxy-7-phenyl-4-quinolinyl)oxy]phenyl]-,
 ethyl ester (CA INDEX NAME)

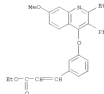


20 828360-24-9 CAPLOS
 CN 2-Propenoic acid,
 3-[4-[(1-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)



20 828360-25-6 CAPLOS
 CN 2-Propenoic acid, 3-[3-[(1-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)



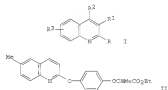
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR
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 FORMAT

L4 ANSWER 3 OF 5 CAPLOS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991398123 CAPLOS
 DOCUMENT NUMBER: 91398123
 ORIGINAL REFERENCE NO.: 91398124,31344
 TITLE: Quinolinesulfonylpropionic acid derivatives and their use as herbicides
 INVENTOR(S): Haeberle A., G., Fed. Rep. Ger.
 PATENT ASSIGNER(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 25 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3101544	A1	19920919	DE 1993-3101544	19930120

PRIORITY APPL. INFO.:
 OTHER SOURCE(S): CASREACT 91398123
 CI

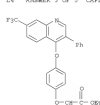


AS 1 [one of R or R2, especially R = 4-(2-OCMeCO2H)34 = CO2H or a derivative, e.g.
 anilide] and the other = H, Cl-4 alkyl, Ph, Cl, Br; R2 = H, Cl-4 alkyl, Cl,
 Br, cyano, Cl-4 carbalkoxy; R3 = H, Cl-4 alkyl, alkoxy, or dialkylamino,
 NO2, CF3, halogen or C=O were prepared as herbicides. Thus, 21 g
 4-(2-OCMeCO2H)34 were added dropwise to 2.3 g NaH in 100 ml DMF, 17.7 g
 2-chloro-4-methylquinoline added, and the mixture was stirred 2 h at
 100° to give 89.23 g.

IT 83948-19
 R1: ACS (Agricultural use); RAC (Biological activity or effector, except
 adenosine); RBT (Biological study, nonclassical); RSP (Synthetic
 preparation); RUC (Biological study); RUS (Preparation); RUS (Use)
 (preparation of, as herbicide)

20 83948-20-3 CAPLOS
 CN Propanoic acid, 2-[4-[(1-ethyl-7-(trifluoromethyl)-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 3 OF 5 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)



[illegible]


14 PAGE 24 OF 5 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)

ANEMER 4 OF CASPUF COPIRIGHT 2009 ACS on STMH (Continued)


(decompr.). 4-*tert*-butyl-1-*l* (20 g.), 9.3 g. *EtOH*, and 40 g. *PhOH* refluxed 4 h., the mixt. heated strongly with 200 cc. *NaOH* and acid. with *HClO*, the mat. evapor., and the residue washed with 200 cc. *NaOH* and decanted, from 95% *EtOH* yielded 39.8 g. of 4-*tert*-butyl-1-*l* in colorless crystals, *m.* 123.4° (from 95% *EtOH*). *Yield* 19.36 g. of 1-*l* added to *NaOH* to make 1.38 g. *Na* in *Liq. NH₃*, the mixt. stirred 5 min., treated with 8.16 g. *EtOH* in *EtOH*, and stirred 1.5 h., the *NaH* evaporated, the *EtOH* suspension refluxed 9 h., dried, with *EtOH*, and filtered, the solid recrystallized from *EtOH* yielded 6.4 g. 4-*tert*-butoxy-1-*l* (*VIII*) of 91, orange plates, *m.* 105.6° (from *EtOH*). *Yield* 17.6 g. of 1-*l* and 2.5 h. at 155° with 70 g. 11, the mixt. decanted, with *EtOH* and filtered, the residue suspended in 120 cc. *N* *NaOH* and acid. with *HClO*, the mat. evapor., and the residue recrystallized from 95% *EtOH* yielded 1.60 g. 4-*tert*-butoxy-2-phenyl ether (*IX*) of 91, light yellow crystals, *m.* 207.9°. 1X hydrolyzed with *HCl* gave 1217B) *NaOH* acid. (X) of 91-phenyl[eth]anone (*IX*). The crude solid (19.9 g.) from *VIII* and 2.1 and refluxed with 5% 40% *EtOH*, 20 cc. *EtOH*, and 5 cc. *NaOH* 7 h. with stirring, the mixt. neutralized with *HClO* and filtered, and the solid washed with *EtOH* and *EtOAc* and triturated with hot *EtOH* gave 2.38 g. *h.* 74% (decolor.) sublimed, *X* (0.25 g.) heated with 50 g. *Et* in dust to red heat and the distillate (collected on the wall of the condensing tube) sublimed at 160° and 0.4 mm. and recrystallized from *EtOH* gave *XI*, *m.* 146.6°.

27 650-65-27, Quinaldine, 4-phenacyl-3-phenyl- 652972-11-7F
Acetophenone, 2-(4-phenacyl-3-phenyl-2-quinyl)-
US 7082 Preparation of

27 650-65-28 2-*l* 652972-11-7F
CH Quinoline, 2-methyl-4-phenacyl-3-phenyl- (A 3188 NAME)



27 652972-11-7F CASPUF
CH Acetophenone, 2-(4-phenacyl-3-phenyl-2-quinyl)- (SC2) (A 3188 NAME)



[illegible]

04/17/2008

10-598,246.trn

L4 ANEMER 1 OF 5 CAPSULE COPYRIGHT 2009 ACS on JTN (Continued)
mol. PANE2 gave 598 V; 0.02 mol. I and 0.04 mol. PANE2 gave 58 V, 228 IV,
and 1.7 g. (PANE)2CO. The PANEClCIPhCO2Et (from 3.8 g. I and 1.7 g.
PANE2), cyclized in 25 or 60 sec. H2O2, gives 47 and 58 V, resp.
IT 860719-92-2Pr Quinoline, 6-chloro-4-phenoxy-3-phenyl-
N: PREP (Preparation)
(separation of)
MI 860719-92-2 CAPSULE
CH Quinoline, 6-chloro-4-phenoxy-3-phenyl- (CA INDEX NAME)



04/17/2008

10-598,246.trn

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	43.57	223.06
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	ENTRY	SESSION
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NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom
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NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
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predefined hit display formats

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=> FIL REGISTRY

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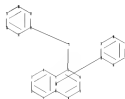
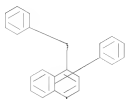
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=>

Uploading C:\Program Files\Stnexp\Queries\10-598,246a.str



chain nodes :

23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22

chain bonds :

7-23 22-23

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

04/17/2008

10-598,246.trn

exact/norm bonds :

7-23 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

isolated ring systems :

containing 1 : 11 : 17 :

G1:O,S

Match level :

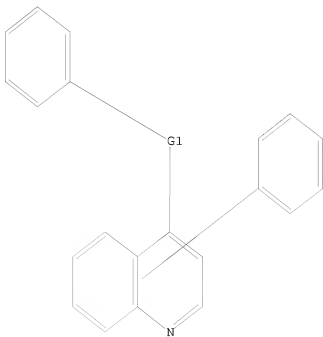
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS 26:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using SIN Express query preparation.

=> s ll sss sam

SAMPLE SEARCH INITIATED 14:52:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 469 TO ITERATE

100.0% PROCESSED 469 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8081 TO 10679

PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s ll sss full

FULL SEARCH INITIATED 14:52:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9410 TO ITERATE

100.0% PROCESSED 9410 ITERATIONS

105 ANSWERS

SEARCH TIME: 00.00.01

L3 105 SEA SSS FUL L1

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SINCE FILE

TOTAL

ENTRY

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179.03

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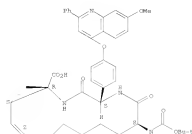
L4 25 L3

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 25 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2008 ACS ON SYN
 ACCESSION NUMBER: 149128256
 DOCUMENT NUMBER: 149128256
 TITLE: Effects on protease inhibition by modifying of helix residues in hepatitis C virus nonstructural protein 3
 AUTHOR(S): Sakl, Göran; Sandström, Anja; Åkerblom, Eva; Danielson, U. Helena
 CORPORATE SOURCE: Department of Biochemistry and Organic Chemistry, Uppsala University, Sweden
 SOURCE: FEBS Journal (2007), 274(22), 5979-5986
 COUNTRY: PRC;N; ISSN: 1742-044X
 SOURCE: Blackwell Publishing Ltd
 PUBLISHER: Journal
 DOCUMENT TYPE: JOURNAL
 LANGUAGE: English
 AB This study of the full-length bifunctional nonstructural protein 3 from hepatitis C virus (HCV) has revealed that residues in the helix domain affect the inhibition of the protease. Two residues (G516 and H520), apparently located in the interface between the 22 and 54 binding pockets of the substrate binding site of the protease, were selected for modification, and three enzyme variants (G516A, H520A and H520S) were expressed, purified and characterized. The substitutions resulted in indistinguishable K_m values and slightly lower k_{cat} values compared to the wild-type. The K_i values for a series of structurally diverse protease inhibitors were affected by the substitutions, with increases or decreases up to 10-fold. The inhibition profiles for H520A and H520S were different, confirming that not only did the removal of the imidazole side chain have an effect, but also that minor differences in the nature of the introduced side chain influenced the characteristics of the enzyme. These results indicate that residues in the helix domain of nonstructural protein 3 can influence the protease, supporting our hypothesis that full-length hepatitis C virus nonstructural protein 3 should be used for protease inhibitor optimization and characterization. Furthermore, the data suggest that inhibitors can be designed to interact with residues in the helix domain, potentially leading to more potent and selective agents.
 IT 1001311-19-0
 RI AMZ (Analytical role, unclassified); B20 (Biological study, unclassified); AMST (Analytical study); B10L (Biological study)
 CH Carboxamide, N-[(1S)-1-[[[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000,1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,1013,1014,1015,1016,1017,1018,1019,1020,1021,1022,1023,1024,1025,1026,1027,1028,1029,1030,1031,1032,1033,1034,1035,1036,1037,1038,1039,1040,1041,1042,1043,1044,1045,1046,1047,1048,1049,1050,1051,1052,1053,1054,1055,1056,1057,1058,1059,1060,1061,1062,1063,1064,1065,1066,1067,1068,1069,1070,1071,1072,1073,1074,1075,1076,1077,1078,1079,1080,1081,1082,1083,1084,1085,1086,1087,1088,1089,1090,1091,1092,1093,1094,1095,1096,1097,1098,1099,1100,1101,1102,1103,1104,1105,1106,1107,1108,1109,1110,1111,1112,1113,1114,1115,1116,1117,1118,1119,1120,1121,1122,1123,1124,1125,1126,1127,1128,1129,1130,1131,1132,1133,1134,1135,1136,1137,1138,1139,1140,1141,1142,1143,1144,1145,1146,1147,1148,1149,1150,1151,1152,1153,1154,1155,1156,1157,1158,1159,1160,1161,1162,1163,1164,1165,1166,1167,1168,1169,1170,1171,1172,1173,1174,1175,1176,1177,1178,1179,1180,1181,1182,1183,1184,1185,1186,1187,1188,1189,1190,1191,1192,1193,1194,1195,1196,1197,1198,1199,1200,1201,1202,1203,1204,1205,1206,1207,1208,1209,1210,1211,1212,1213,1214,1215,1216,1217,1218,1219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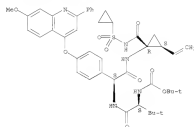
L4 ANMER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



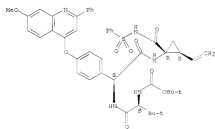
2T 928162-36-1P 928162-37-2P 928162-38-3P
 928162-39-4P 928162-40-7P 928162-41-1P
 928162-42-4P 928162-43-1P 928162-44-1P
 928162-45-7P
 324.266 (Drug mechanism of action); PAC (Pharmacological activity); SYN (Synthetic preparation); THO (Therapeutic use); BIOB (Biological study); PREP (Preparation); UNES (Uses)
 Hepatitis C virus NS3 protease inhibitors preparation; phenylglyoxime
 as novel 22 scaffold
 2H 928162-36-1 CAPLUS
 CH Cyclopropanecarboxamide,
 N-[(1,2-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)
 Absolute stereochemistry.

L4 ANMER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

Absolute stereochemistry.

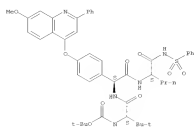


2H 928162-39-4 CAPLUS
 CH Cyclopropanecarboxamide,
 N-[(1,2-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)
 Absolute stereochemistry.

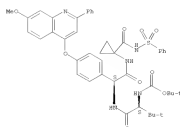


2H 928162-40-7 CAPLUS
 CH Butanamide, N-[(1,2-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-4,4-difluoro-, (2S)- (CA INDEX NAME)
 Absolute stereochemistry.

L4 ANMER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



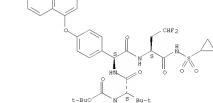
2H 928162-37-2 CAPLUS
 CH Cyclopropanecarboxamide,
 N-[(1,2-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(phenylsulfonyl)- (CA INDEX NAME)
 Absolute stereochemistry.



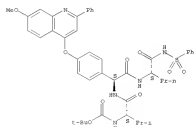
2H 928162-38-3 CAPLUS
 CH Cyclopropanecarboxamide,
 N-[(1,2-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)
 Absolute stereochemistry.

L4 ANMER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

Absolute stereochemistry.

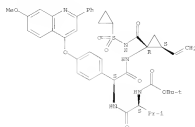


2H 928162-46-3 CAPLUS
 CH L-Valinalanide, N-[(1,2-dimethylethoxy)carbonyl]-4-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)
 Absolute stereochemistry.



2H 928162-41-4 CAPLUS
 CH Cyclopropanecarboxamide, N-[(1,2-dimethylethoxy)carbonyl]-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyloxy)phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)
 Absolute stereochemistry.

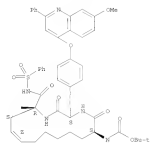
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



NN 928162-60-1 CAPLUS

CH Carboxylic acid, N-[[13,45,78,132,155]-4-[4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]-7,6-dioxo-1-[[phenylamino]amino]carboxyl]-2,5-dioxabicyclo[13.1.0]hexadec-13-en-7-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

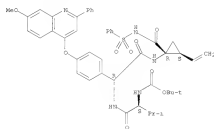
Absolute stereochemistry.
Double bond geometry as shown.



NN 928162-61-2 CAPLUS

CH Carboxylic acid, N-[[13,45,78,132,155]-3-[[cyclopropylsulfonyl]amino]carboxyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



IT 928162-13-4P 928162-18-8P 928162-19-0P

928162-20-3P 928162-21-4P 928162-25-8P

928162-26-8P 928162-27-0P 928162-28-1P

928162-29-2P 928162-51-0P 928162-54-3P

945901-18-7P 945901-18-8P 945901-91-0P

945901-14-6P 945901-18-8P 945901-32-0P

NA KCT (Reagent); SPH (Synthetic preparation); PREP (Preparation); ROCT (Reagent or reagent)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

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as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

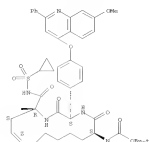
as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

as (Bepatitis C virus NS3 protease inhibitors preparation; phenylglycine)

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
yl)-4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]-7,6-dioxo-2,5-dioxabicyclo[13.1.0]hexadec-13-en-7-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



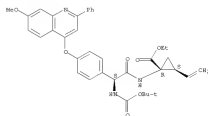
NN 928162-66-7 CAPLUS

CH Cyclopropylcarboxylic acid, N-[[1,1,3-dimethylethoxy]carboxyl]-4-valyl-(1R)-2-[4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]glycyl]-1-amino-2-ethenyl-5-quinolinyloxy]-, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
dimethylethoxy]carboxyl]amino]-2-[4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]acetyl]amino]-4,6-difluoro-, ethyl ester, (2S)- (CA INDEX NAME)

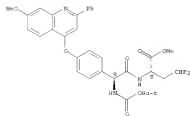
Absolute stereochemistry.



NN 928162-19-0 CAPLUS

CH Butanoic acid, 2-[[12R)-2-[[1,1,3-dimethylethoxy]carboxyl]amino]-2-[4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]acetyl]amino]-4,6-difluoro-, methyl ester, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

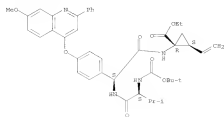


NN 928162-20-3 CAPLUS

CH Cyclopropylcarboxylic acid, N-[[1,1,3-dimethylethoxy]carboxyl]-4-valyl-(1R)-2-[4-[[17-methoxy-2-phenyl-4-quinolinyloxy]phenyl]glycyl]-1-amino-2-ethenyl-5-quinolinyloxy]-, ethyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.

14 ANSMER 2 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)

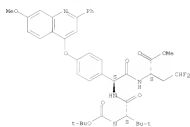


RN 928162-21-4 CAPLOS

CN Carbamic acid,

N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-1-valyl-(2S)-2-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]glycyl-2-amino-4,4-difluoro-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



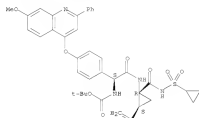
RN 928162-21-5 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-2-oxo-2-[1-(2S)-2-[[1-(phenylsulfonyl)amino]carbonyl]butyl]amino]ethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

14 ANSMER 2 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)

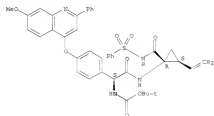


RN 928162-28-1 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

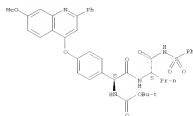


RN 928162-29-2 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

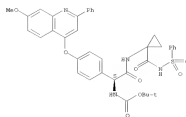
14 ANSMER 2 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)
Absolute stereochemistry.

RN 928162-26-9 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



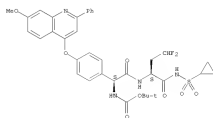
RN 928162-27-0 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

14 ANSMER 2 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)

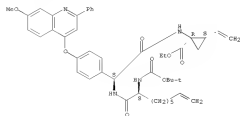


RN 928162-31-0 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



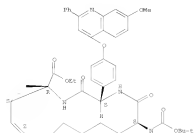
RN 928162-34-3 CAPLOS

CN Carbamic acid,

N-[(1S)-2-[[1-(1S,2S)-2-ethoxy-1-[[1-(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]-2-oxoethyl]-1,1-dimethylethyl ester (CA INDEX NAME)

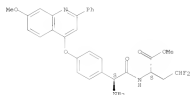
Absolute stereochemistry.
Double bond geometry as shown.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN (Continued)



RI 94594-19-7 CAPLUS
 CH Butanoic acid, 2-[[[(2S)-2-amino-2-[4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]acetyl]amino]-4,4-difluoro-1-methyl-ester], (2S)- (CA INDEX NAME)

Absolute stereochemistry.

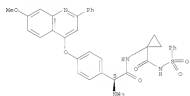


RI 94594-33-9 CAPLUS
 CH Benzenecarboxamide, N-amino-4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]-N-[[[8-[[[1-[[[phenyl]sulfonyl]amino]carboxyl]oxy]sty]-, hydrochloride (1:1), (aS)- (CA INDEX NAME)

Absolute stereochemistry.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN (Continued)

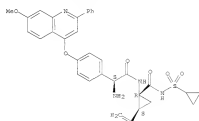
Absolute stereochemistry.



● IC1

RI 94595-14-8 CAPLUS
 CH Benzenecarboxamide, N-amino-4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]-N-[[[8-[[[1-[[[phenyl]sulfonyl]amino]carboxyl]oxy]sty]-, hydrochloride (1:1), (aS)- (CA INDEX NAME)

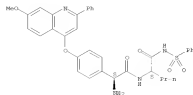
Absolute stereochemistry.



● IC1

RI 94595-32-9 CAPLUS
 CH Benzenecarboxamide, N-amino-4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]-N-[[[8-[[[1-[[[phenyl]sulfonyl]amino]carboxyl]oxy]sty]-, hydrochloride (1:1), (aS)- (CA INDEX NAME)

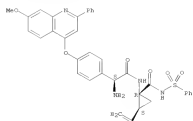
14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN (Continued)



● IC1

RI 94594-95-0 CAPLUS
 CH Benzenecarboxamide, N-amino-4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]-N-[[[8-[[[1-[[[phenyl]sulfonyl]amino]carboxyl]oxy]sty]-, hydrochloride (1:1), (aS)- (CA INDEX NAME)

Absolute stereochemistry.

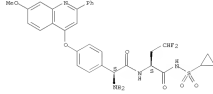


● IC1

RI 94595-14-4 CAPLUS
 CH Benzenecarboxamide, N-amino-4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]-N-[[[8-[[[1-[[[phenyl]sulfonyl]amino]carboxyl]oxy]sty]-, hydrochloride (1:1), (aS)- (CA INDEX NAME)

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN (Continued)

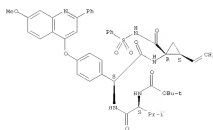
Absolute stereochemistry.



● IC1

IT 929162-65-6P
 RI: SYN (Synthetic preparation); PREP (Preparation)
 CH Hepatitis C virus NS5 protease inhibitors preparations: phenylglycine as novel P2 covalent
 RI 929162-65-6 CAPLUS
 CH Cyclohexanecarboxamide, N-[[[1,1-dimethylethoxy]carboxyl]-4-valyl]-2-[[4-[[[7-methoxy-2-phenyl-4-quinolinyl]oxy]phenyl]glycyl-1-amino-2-ethoxy-1-phenyl]sulfonyl], (1S,2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS ARE IN THE RECORD.

FORMAT

04/17/2008

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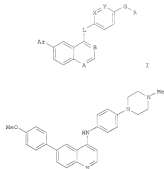
14 NUMBER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AL4 MEMBER 3 OF 21 CAPLUS COPYRIGHT 2008 ACS on STM
ACCESSION NUMBER: 1444-675959 CAPLUS
DOCUMENT NUMBER: 1444-675746
TITLE: Preparation of quinoline and laquinomoline-based compounds exhibiting ATP-utilizing enzyme inhibitory activity, and compositions, and uses thereof
INVENTOR(S): Dickson, John E., Jr.; Williams, Kevin P.; Hodge, Carl
PATENT ASSIGNER(S): Nicholas
SOURCE: Amphora Bioscience Corporation, OMA
COUNTRY: USA
COINSTR: P14363
PUBINT: Patent
FAMILY AC. NUM. COVERED: 1
LAWFIRM INFORMATION: American Information

PATIENT NO.		KIND DATE	APPLICATION NO.	DATE
NO 2005120507		A	20051222	NO 2005-0319255
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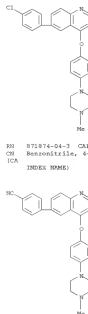
OTHER SOURCE(S): CASREACT 144:60746; NARPAT 144:60746
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14 ANSWER 3 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Cont. Speed)

[illegible]

871874-03-2 CAPLUS

L4 ANSWER 3 OF 25 CAPLOS COPYRIGHT 2008 ACS on STM (Continued)
CN Quinoline, 6-[4-chlorophenyl]-4-[4-(4-methyl-1-piperazinyl)phenoxy]- (CA
INDEX NAME)



REFERENCE COURT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

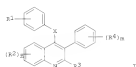
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14  ANIMAR 4 OF 2  CAPRUS  CAPRUS 2005 ACS on STN
ACCESSION NUMBER: 20051979616 CAPRUS
SEQUENCE NUMBER: 14126850
TITLE: Preparation of substituted quinoline compounds for
use
as selective estrogen receptor modulator
INVENTOR(S): Boekstra, William Joel; Miller, Aaron Bayne;
Czechowicz,
William John; Patel, Barikashna Daryankant
PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA
SOURCE: Pub. Int. Appl., 42 pp.
CODING: P14103
SEQUENCE TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PARENT INFORMATION:

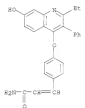
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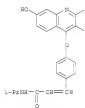
OTHER SOURCE(S): CASREACT 143:266830; NAFPAT 143:266830



14 ANSWER 4 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)



3-[4-[[2-ethyl-1-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-
N-(1-methylethyl)- (CA INDEX NAME)



IN 829300-10-3 CAPLUS
 CN 2-Pregnenolone,
 3-[4-[(2-ethyl-1-hydroxy-3-phenyl-4-quinolanyl)oxy]phenyl]-
 N,N-dimethyl- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STM (Continued)

AB The present invention relates to novel compds. of Formula (I, variables defined below) with a variety of therapeutic uses, more particularly

substituted quinoline compounds, particularly useful for selective estrogen receptor modulation. For 1, the variables are: R1 = CH₃-CH₂-R⁵, R⁵ = CH₃, C10H₇, C10H₈-R1(R⁷); R⁶ and R⁷ = H, alkyl, aryl; or R⁶ and R⁷ may combine with the R1 to which they are attached to form a 3 to 7 membered ring; R⁸ may be substituted or unsubstituted ring; R⁹ = H, alkyl, aryl, haloalkyl, hydroxy, alkoxy, aryloxy, aralkyloxy, alkoxyaralkyloxy, arylalkoxyaralkyloxy, aralkyloxyaralkyloxy, alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or selenoyloxy; n = 1 or 2; R¹⁰ = H, CH₃, C10H₇, C10H₈, alkoxy, aralkoxy, aralkoxyalkoxy, aralkoxyalkoxyalkoxy, haloalkyl, alkyl, aryl, heteroalkyl, aralkyl, or heteroalkyl; X = S, O, Si, SO₂.

or
SiO₂; each R⁴ independently = H, halogen, haloalkyl, OH, alkoxy,
aryloxy,
alkoxyloxy, alkoxycarbonyloxy, aryloxy carbonyloxy, aralkyloxy carbonyloxy,
alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or acyloxy; and m
= 1 or 2.

17 828300-07-8P 828300-08-9P 828300-09-0P
828300-10-3P 828300-11-4P 828300-12-5P
828300-13-6P 828300-14-7P 863711-16-6P
863711-17-5P 863711-18-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BICL (Biological study); PREP (Preparation); USSS

selective estrogen receptor modulator to treat various diseases)

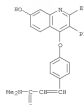
723 826300-07-8 CAPLOS

CN 2-Propenoic acid, 3-[4-[[2-ethyl-7-hydroxy-3-phenyl-4-quinolinylmethyl]phenyl]- (CA INDEX NAME)

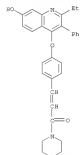


HN 828700-08-9 CAPLOS
 CN 2-Propenamide,
 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]

14 ANSWER 4 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)



IN 028300-11-4 CAPLUS
 CN Piperidine,
 1-[3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-
 1-oxo-2-propenyl]- (PCI) (CA INDEX NAME)

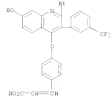


KN 828300-12-5 CAPLUS
CN 2-Propenoic acid,
3-[4-[[7-hydroxy-2,3-diphenyl-4-quinolinsyl)oxy]phenyl]-
(CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

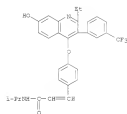


RI 828300-13-6 CAPLUS
 CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

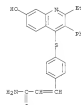


RI 828300-14-7 CAPLUS
 CH 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 863711-19-6 CAPLUS
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]- (CA INDEX NAME)



IT 863711-19-7
 RI: RCT (Reactant); RACT (Reactant or reagent)
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]- (Preparation of substituted quinoline compounds. For use as selective estrogen receptor modulator to treat various diseases)
 RI 863711-19-7 CAPLUS
 CH 7-Quinolinsulfonyl, 4-(4-bromophenoxy)-2-ethyl-3-phenyl- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 863711-16-4 CAPLUS
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



RI 863711-17-5 CAPLUS
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



IT 828300-18-1F, 2-Ethyl-3-phenyl-4-(4-bromophenoxy)-7-methoxyquinoline 828300-22-7F
 RI: RCT (Reactant); RACT (Reactant or reagent); PREP (Preparation); RACT (Reactant or reagent)
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]- (Preparation of substituted quinoline compounds. For use as selective estrogen receptor modulator to treat various diseases)
 RI 828300-18-1 CAPLUS
 CH Quinolinsulfonyl, 4-(4-bromophenoxy)-2-ethyl-3-phenyl- (CA INDEX NAME)



RI 828300-22-7 CAPLUS
 CH 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]-, ethyl ester (CA INDEX NAME)

[illegible]

IT	Peptide profile of constrained triamides were compared to known proliferative and nonproliferative ER ligands to discover potent quinoxaline-based ligands with minimal Ishikawa cell stimulation.
	828300-67-9; 828300-68-9; 828300-69-0; 828300-71-0; 828300-72-0; 828300-73-0; 828300-74-9; 828300-75-0; 828300-76-0; 828300-77-0; 828300-78-0; 828300-79-0; 828300-80-0; 828300-81-0; 828300-82-0; 828300-83-0; 828300-84-0; 828300-85-0; 828300-86-0; 828300-87-0; 828300-88-0; 828300-89-0; 828300-90-0; 828300-91-0; 828300-92-0; 828300-93-0; 828300-94-0; 828300-95-0; 828300-96-0; 828300-97-0; 828300-98-0; 828300-99-0; 828300-100-0; 828300-101-0; 828300-102-0; 828300-103-0; 828300-104-0; 828300-105-0; 828300-106-0; 828300-107-0; 828300-108-0; 828300-109-0; 828300-110-0; 828300-111-0; 828300-112-0; 828300-113-0; 828300-114-0; 828300-115-0; 828300-116-0; 828300-117-0; 828300-118-0; 828300-119-0; 828300-120-0; 828300-121-0; 828300-122-0; 828300-123-0; 828300-124-0; 828300-125-0; 828300-126-0; 828300-127-0; 828300-128-0; 828300-129-0; 828300-130-0; 828300-131-0; 828300-132-0; 828300-133-0; 828300-134-0; 828300-135-0; 828300-136-0; 828300-137-0; 828300-138-0; 828300-139-0; 828300-140-0; 828300-141-0; 828300-142-0; 828300-143-0; 828300-144-0; 828300-145-0; 828300-146-0; 828300-147-0; 828300-148-0; 828300-149-0; 828300-150-0; 828300-151-0; 828300-152-0; 828300-153-0; 828300-154-0; 828300-155-0; 828300-156-0; 828300-157-0; 828300-158-0; 828300-159-0; 828300-160-0; 828300-161-0; 828300-162-0; 828300-163-0; 828300-164-0; 828300-165-0; 828300-166-0; 828300-167-0; 828300-168-0; 828300-169-0; 828300-170-0; 828300-171-0; 828300-172-0; 828300-173-0; 828300-174-0; 828300-175-0; 828300-176-0; 828300-177-0; 828300-178-0; 828300-179-0; 828300-180-0; 828300-181-0; 828300-182-0; 828300-183-0; 828300-184-0; 828300-185-0; 828300-186-0; 828300-187-0; 828300-188-0; 828300-189-0; 828300-190-0; 828300-191-0; 828300-192-0; 828300-193-0; 828300-194-0; 828300-195-0; 828300-196-0; 828300-197-0; 828300-198-0; 828300-199-0; 828300-200-0; 828300-201-0; 828300-202-0; 828300-203-0; 828300-204-0; 828300-205-0; 828300-206-0; 828300-207-0; 828300-208-0; 828300-209-0; 828300-210-0; 828300-211-0; 828300-212-0; 828300-213-0; 828300-214-0; 828300-215-0; 828300-216-0; 828300-217-0; 828300-218-0; 828300-219-0; 828300-220-0; 828300-221-0; 828300-222-0; 828300-223-0; 828300-224-0; 828300-225-0; 828300-226-0; 828300-227-0; 828300-228-0; 828300-229-0; 828300-230-0; 828300-231-0; 828300-232-0; 828300-233-0; 828300-234-0; 828300-235-0; 828300-236-0; 828300-237-0; 828300-238-0; 828300-239-0; 828300-240-0; 828300-241-0; 828300-242-0; 828300-243-0; 828300-244-0; 828300-245-0; 828300-246-0; 828300-247-0; 828300-248-0; 828300-249-0; 828300-250-0; 828300-251-0; 828300-252-0; 828300-253-0; 828300-254-0; 828300-255-0; 828300-256-0; 828300-257-0; 828300-258-0; 828300-259-0; 828300-260-0; 828300-261-0; 828300-262-0; 828300-263-0; 828300-264-0; 828300-265-0; 828300-266-0; 828300-267-0; 828300-268-0; 828300-269-0; 828300-270-0; 828300-271-0; 828300-272-0; 828300-273-0; 828300-274-0; 828300-275-0; 828300-276-0; 828300-277-0; 828300-278-0; 828300-279-0; 828300-280-0; 828300-281-0; 828300-282-0; 828300-283-0; 828300-284-0; 828300-285-0; 828300-286-0; 828300-287-0; 828300-288-0; 828300-289-0; 828300-290-0; 828300-291-0; 828300-292-0; 828300-293-0; 828300-294-0; 828300-295-0; 828300-296-0; 828300-297-0; 828300-298-0; 828300-299-0; 828300-300-0; 828300-301-0; 828300-302-0; 828300-303-0; 828300-304-0; 828300-305-0; 828300-306-0; 828300-307-0; 828300-308-0; 828300-309-0; 828300-310-0; 828300-311-0; 828300-312-0; 828300-313-0; 828300-314-0; 828300-315-0; 828300-316-0; 828300-317-0; 828300-318-0; 828300-319-0; 828300-320-0; 828300-321-0; 828300-322-0; 828300-323-0; 828300-324-0; 828300-325-0; 828300-326-0; 828300-327-0; 828300-328-0; 828300-329-0; 828300-330-0; 828300-331-0; 828300-332-0; 828300-333-0; 828300-334-0; 828300-335-0; 828300-336-0; 828300-337-0; 828300-338-0; 828300-339-0; 828300-340-0; 828300-341-0; 828300-342-0; 828300-343-0; 828300-344-0; 828300-345-0; 828300-346-0; 828300-347-0; 828300-348-0; 828300-349-0; 828300-350-0; 828300-351-0; 828300-352-0; 828300-353-0; 828300-354-0; 828300-355-0; 828300-356-

14 ANSWER 7 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)



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      \begin{array}{c}
\text{1-Propyl}-\text{C}\equiv\text{CH} \\
| \\
\text{O}
\end{array}

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P01 826700-10-3 CAPLUS
 CN 2-Propenamide,
 3-[4-{[2-ethyl-3-(ethoxy-3-pheryl-4-quinoxalinyloxy)phenyl]-
 N,N-dimethyl- (CA INDEX NAME)}

CC1=CC=C(C=C1)C(=O)N2C=CC=CC=C2

L4 ANSWER 7 OF 25 CAPLES COPYRIGHT 2008 ACS on STM (Continued)



$\text{HO}_2\text{C}-\text{CH}=\text{CH}$
 722 828100-08-9 CAP105
 CN 2-Propenamide,
 3-[4-[(2-ethyl-7-hydroxy-7-phenyl-1-4-quinolinyl)oxy]phenyl]-
 (CA INDEX NAME)

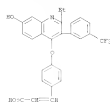

$$\text{R}_2\text{N}-\overset{\text{O}}{\underset{\text{O}}{\text{C}}}-\text{CH}=\text{CH}_2$$

FN 826300-09-0 CAPLOS
 CN 2-Propenenide,
 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-
 N-(1-methylethyl)- (CA INDEX NAME)

1.4 ANSWER 7 OF 25 CASLOS COPYRIGHT 2008 ACS on STN (Continued)

C=CC(=O)N1CCCC1HO2C-C#C-c1ccc(OCC2=CC=CC=C2)cc1

14 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 828700-14-7 CAPLUS
 CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl)-4-quinolinyl]oxy]phenyl- (CA INDEX NAME)



HN 828700-15-8 CAPLUS
 CN 7-Quinolone, 4-[4-[(2-dimethylamino)ethoxy]phenyl]-2-ethyl-3-phenyl- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



17 828700-18-1P 828700-19-2P 828700-20-5P
 828700-21-4P 828700-22-7P 828700-23-8P
 R1: RCT (Reagent); R1P (Synthetic Preparation); PREP (Preparation); R1CT (Reagent or reagent)
 (discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)
 HN 828700-18-1 CAPLUS
 CN Quinolone, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)

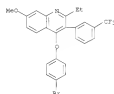


HN 828700-19-2 CAPLUS
 CN Quinolone, 4-(4-bromophenoxy)-7-methoxy-2,3-diphenyl- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 828700-20-5 CAPLUS
 CN Quinolone, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



HN 828700-21-6 CAPLUS
 CN Quinolone, 4-(3-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



HN 828700-22-7 CAPLUS
 CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl)-4-quinolinyl]oxy]phenyl- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

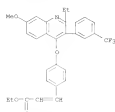


HN 828700-23-8 CAPLUS
 CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl)-4-quinolinyl]oxy]phenyl- (CA INDEX NAME)

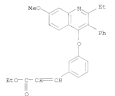


HN 828700-24-9 CAPLUS
 CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl)-4-quinolinyl]oxy]phenyl- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STM (Continued)



NO 200700121-6 CAPLUS
 CH 2-Propenoic acids, 2-[3-[[2-ethyl-7-methoxy-3-phenyl-4-quinoxalylidene]phenyl]-, ethyl ester (CA INDEX NAME)



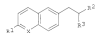
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

14 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STM (Continued)

OTHER SOURCE(S): MARPAT 139181384

CI



AS Title compds. I | X = H, CH; XI = XI = cycloalkyl, aryl, heterocyclic, heterocycloalkyl, substituted CN, carbonyl-1-yl; Z = (un)substituted H₂, CH, CO₂R₁, Z = 2,6-dichlorophenyl, Z = H₂, CH, CO₂R₁. This compound was prepared for use in treating VLA-4 dependent inflammatory disease such

as asthma, allergic rhinitis, sinusitis, conjunctivitis, food allergy, psoriasis, urticaria, pruritus, eczema, rheumatoid arthritis, inflammatory bowel disease, multiple sclerosis and atherosclerosis (no data). Thus, 4-nitrophenylamine was esterified, 3-pyrenylated, reduced to the amine, cyclized with 2,6-dichlorophenyl and CH₂Cl₂/PPh₃, followed by elimination of PPh₃ to give I (X = H, XI = 2,6-dichlorophenyl, Z = H₂, CH, CO₂R₁). This compound was deprotected and acylated with 2,6-dichlorophenyl, followed by ester hydrolysis to give II (X = H, XI = 2,6-dichlorophenyl, Z = 2,6-dichlorophenyl).

R₁ = CO₂R₁R₂ = CO₂R₁R₃ = CO₂R₁R₄ = CO₂R₁R₅ = CO₂R₁R₆ = CO₂R₁R₇ = CO₂R₁R₈ = CO₂R₁R₉ = CO₂R₁R₁₀ = CO₂R₁R₁₁ = CO₂R₁R₁₂ = CO₂R₁R₁₃ = CO₂R₁R₁₄ = CO₂R₁R₁₅ = CO₂R₁R₁₆ = CO₂R₁R₁₇ = CO₂R₁R₁₈ = CO₂R₁R₁₉ = CO₂R₁R₂₀ = CO₂R₁R₂₁ = CO₂R₁R₂₂ = CO₂R₁R₂₃ = CO₂R₁R₂₄ = CO₂R₁R₂₅ = CO₂R₁R₂₆ = CO₂R₁R₂₇ = CO₂R₁R₂₈ = CO₂R₁R₂₉ = CO₂R₁R₃₀ = CO₂R₁R₃₁ = CO₂R₁R₃₂ = CO₂R₁R₃₃ = CO₂R₁R₃₄ = CO₂R₁R₃₅ = CO₂R₁R₃₆ = CO₂R₁R₃₇ = CO₂R₁R₃₈ = CO₂R₁R₃₉ = CO₂R₁R₄₀ = CO₂R₁R₄₁ = CO₂R₁R₄₂ = CO₂R₁R₄₃ = CO₂R₁R₄₄ = CO₂R₁R₄₅ = CO₂R₁R₄₆ = CO₂R₁R₄₇ = CO₂R₁R₄₈ = CO₂R₁R₄₉ = CO₂R₁R₅₀ = CO₂R₁R₅₁ = CO₂R₁R₅₂ = CO₂R₁R₅₃ = CO₂R₁R₅₄ = CO₂R₁R₅₅ = CO₂R₁R₅₆ = CO₂R₁R₅₇ = CO₂R₁R₅₈ = CO₂R₁R₅₉ = CO₂R₁R₆₀ = CO₂R₁R₆₁ = CO₂R₁R₆₂ = CO₂R₁R₆₃ = CO₂R₁R₆₄ = CO₂R₁R₆₅ = CO₂R₁R₆₆ = CO₂R₁R₆₇ = CO₂R₁R₆₈ = CO₂R₁R₆₉ = CO₂R₁R₇₀ = CO₂R₁R₇₁ = CO₂R₁R₇₂ = CO₂R₁R₇₃ = CO₂R₁R₇₄ = CO₂R₁R₇₅ = CO₂R₁R₇₆ = CO₂R₁R₇₇ = CO₂R₁R₇₈ = CO₂R₁R₇₉ = CO₂R₁R₈₀ = CO₂R₁R₈₁ = CO₂R₁R₈₂ = CO₂R₁R₈₃ = CO₂R₁R₈₄ = CO₂R₁R₈₅ = CO₂R₁R₈₆ = CO₂R₁R₈₇ = CO₂R₁R₈₈ = CO₂R₁R₈₉ = CO₂R₁R₉₀ = CO₂R₁R₉₁ = CO₂R₁R₉₂ = CO₂R₁R₉₃ = CO₂R₁R₉₄ = CO₂R₁R₉₅ = CO₂R₁R₉₆ = CO₂R₁R₉₇ = CO₂R₁R₉₈ = CO₂R₁R₉₉ = CO₂R₁R₁₀₀ = CO₂R₁R₁₀₁ = CO₂R₁R₁₀₂ = CO₂R₁R₁₀₃ = CO₂R₁R₁₀₄ = CO₂R₁R₁₀₅ = CO₂R₁R₁₀₆ = CO₂R₁R₁₀₇ = CO₂R₁R₁₀₈ = CO₂R₁R₁₀₉ = CO₂R₁R₁₁₀ = CO₂R₁R₁₁₁ = CO₂R₁R₁₁₂ = CO₂R₁R₁₁₃ = CO₂R₁R₁₁₄ = CO₂R₁R₁₁₅ = CO₂R₁R₁₁₆ = CO₂R₁R₁₁₇ = CO₂R₁R₁₁₈ = CO₂R₁R₁₁₉ = CO₂R₁R₁₂₀ = CO₂R₁R₁₂₁ = CO₂R₁R₁₂₂ = CO₂R₁R₁₂₃ = CO₂R₁R₁₂₄ = CO₂R₁R₁₂₅ = CO₂R₁R₁₂₆ = CO₂R₁R₁₂₇ = CO₂R₁R₁₂₈ = CO₂R₁R₁₂₉ = CO₂R₁R₁₃₀ = CO₂R₁R₁₃₁ = CO₂R₁R₁₃₂ = CO₂R₁R₁₃₃ = CO₂R₁R₁₃₄ = CO₂R₁R₁₃₅ = CO₂R₁R₁₃₆ = CO₂R₁R₁₃₇ = CO₂R₁R₁₃₈ = CO₂R₁R₁₃₉ = CO₂R₁R₁₄₀ = CO₂R₁R₁₄₁ = CO₂R₁R₁₄₂ = CO₂R₁R₁₄₃ = CO₂R₁R₁₄₄ = CO₂R₁R₁₄₅ = CO₂R₁R₁₄₆ = CO₂R₁R₁₄₇ = CO₂R₁R₁₄₈ = CO₂R₁R₁₄₉ = CO₂R₁R₁₅₀ = CO₂R₁R₁₅₁ = CO₂R₁R₁₅₂ = CO₂R₁R₁₅₃ = CO₂R₁R₁₅₄ = CO₂R₁R₁₅₅ = CO₂R₁R₁₅₆ = CO₂R₁R₁₅₇ = CO₂R₁R₁₅₈ = CO₂R₁R₁₅₉ = CO₂R₁R₁₆₀ = CO₂R₁R₁₆₁ = CO₂R₁R₁₆₂ = CO₂R₁R₁₆₃ = CO₂R₁R₁₆₄ = CO₂R₁R₁₆₅ = CO₂R₁R₁₆₆ = CO₂R₁R₁₆₇ = CO₂R₁R₁₆₈ = CO₂R₁R₁₆₉ = CO₂R₁R₁₇₀ = CO₂R₁R₁₇₁ = CO₂R₁R₁₇₂ = CO₂R₁R₁₇₃ = CO₂R₁R₁₇₄ = CO₂R₁R₁₇₅ = CO₂R₁R₁₇₆ = CO₂R₁R₁₇₇ = CO₂R₁R₁₇₈ = CO₂R₁R₁₇₉ = CO₂R₁R₁₈₀ = CO₂R₁R₁₈₁ = CO₂R₁R₁₈₂ = CO₂R₁R₁₈₃ = CO₂R₁R₁₈₄ = CO₂R₁R₁₈₅ = CO₂R₁R₁₈₆ = CO₂R₁R₁₈₇ = CO₂R₁R₁₈₈ = CO₂R₁R₁₈₉ = CO₂R₁R₁₉₀ = CO₂R₁R₁₉₁ = CO₂R₁R₁₉₂ = CO₂R₁R₁₉₃ = CO₂R₁R₁₉₄ = CO₂R₁R₁₉₅ = CO₂R₁R₁₉₆ = CO₂R₁R₁₉₇ = CO₂R₁R₁₉₈ = CO₂R₁R₁₉₉ = CO₂R₁R₂₀₀ = CO₂R₁R₂₀₁ = CO₂R₁R₂₀₂ = CO₂R₁R₂₀₃ = CO₂R₁R₂₀₄ = CO₂R₁R₂₀₅

L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
REFERENCE COUNT: 00 THERE ARE 00 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

AN	ANMER 10 OF 10	CAPUSL COPYRIGHT 2008 ACS on STN
AC	ACCESSION NUMBER	132341-50
AD	ADDITIONAL INFORMATION	132341-50
TI	TITLE	Reaction of functionalized quinolones through acid-catalyzed/amination reactions of P- β -aminoanhydride- β - β -proton
AU	AUTHOR(S)	Antonino Ricciardi, Fabio Nesi, Elisabetta
CO	CORPORATE SOURCE	dipartimento di Chimica Inorganica Chimica e
LA	LANGUAGE	English
OR	ORIGIN	La Facoltà di Scienze, Università di L'Aquila, L'Aquila, I-67100, Italy
SO	SOURCE	Tetrahedron (1999), 55(46), 13233-13250
PU	PUBLISHED	CODING TEXT(S) 0010, 0040
DO	DOCUMENT TYPE	Elsevier Science Direct
JA	JANUARY	English
COE	CODING SOURCE	132341-50
AB	ABSTRACT	P- β -aminoanhydride- β - β -proton can quickly give
		rise to a series of functionalized quinolones through acid-catalyzed/amination reactions. Acid-catalyzed cyclization of P- β -aminoanhydride- β - β -proton with 2-aminophenol and 2-aminobenzonitrile gave 2-aminophenol and 2-aminobenzonitrile derivatives. The entry into 4- <i>l</i> -levo-2-substituted quinolones prompted the development of a
		new procedure for synthesis of 4- <i>l</i> -levo-2-substituted quinolones by
		further
		hydrolysis of the corresponding 4- <i>l</i> -levo-2-substituted quinolones. The separate
		basic conditions of use of P- β -aminoanhydride- β - β -proton and the separate
		acid-catalyzed cyclization of P- β -aminoanhydride- β - β -proton led to a fused
		quinolone derivative through intramolecular Michael
		addition. The fused quinolone derivative was cyclized through an acid-catalyzed
		Michael addition to give a fused quinolone derivative. The fused
		polycyclic quinolones can be viewed as occurring through a tandem
		Michael addition. The fused quinolone derivative was cyclized through an
		acid-catalyzed Michael addition to give a fused quinolone derivative. The
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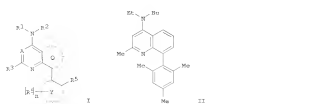
L4 ANSWER 10 OF 25 CAPLOS COPYRIGHT 2008 ACS on STN (Continued)
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

14 ANMERK 11 GF 25 CAPLOS COPYRIGHT 2000 ACS ON STM
ACCESSION NUMBER: 1999-194128 CAPLOS
DOCUMENT NUMBER: 10123763
TITLE: Preparation of spinolone and quinamine derivatives
having corticotropin releasing factor (CRF)
antagonist activity
INVENTOR(S): Den Hartog, Jacobus A. J.; Visszer, Gerben M.; Toorop,
Gerrit P.; Jansen, Johannes W. C. M.; Sonkenen, Errol
Tulp, Martinus Th. J.; Beenders, Jan H.
PATENT APPLICANT(S): Duglar International Research B.V., Neth.
SOURCE: PCT Int. Appl., 24 pp.
CDB#: P194128
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
SUBST. INFORMATION:

[illegible]

OTHER SOURCE(S) :
GT

L4 ANSWER 11 OF 25 CAPLOS COPYRIGHT 2008 ACS ON STN (Continued)



AB The title compounds, [Y = CH, N; Q = (un)substituted Ph, pyridyl, pyrrolidinyl, pyridazinyl; Y = Ph, pyridyl, pyrrolidinyl, etc.; R₁, R₂ = (un)substituted alkyl, alkenyl, alkynyl, etc.; R₃, R₄, alkyl optionally substituted with one or more F atoms; R₅ = halo, MeO, EtO, etc.; R₅ = halo, alkyl, alkenyl, etc.; n = 0-4], having corticotropin releasing factor (CRF) antagonist activity (no data) and useful in the treatment of a wide range of stress related disorders, were prepared. E.g., a 4-step synthesis of quinoline II, starting with 2-methyl-4-hydroxy-6-bromoquinoline, was given.

IT 221295-72-29
 RU ECT (Isosantol); SPN (Synthetic preparation); PREP (Preparation); RACT (Isosantol or reagent)
 Preparation of quinoline and quinazoline deriva. having corticotropin releasing factor (CRF) antagonist activity)
 RU 221295-72-2 CAPLOS
 CH Quinoline, 2-methyl-4-phenoxy-8-[1,4,6-trimethylphenyl]- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

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L4 ANSWER 12 OF 25 CAPLOS COPYRIGHT 2008 ACS ON STN (Continued)

RU 226412-51-2 CAPLOS
 CH Serenoxaline, N-methoxy-3-[(2-phenyl-4-quinolinyl)oxy]- (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 13 OF 25 CAPLOS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1999:1983 CAPLOS
 130162747
 TITLE: Quantitative structure-activity relationship studies on some nonbenzodiazepine series of compounds acting at the benzodiazepine receptor
 AUTHOR(S): Gupta, S. P.; Paletti, Anitha
 CORPORATE SOURCE: Department of Chemistry, Kirti Institute of Technology and Sciences, Kirti, 337 571, India
 SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(11), 2117-2218
 PUBLINE: COORDINATE NUMBER: 0948-0096
 PUBLISHER: Elsevier Science Ltd.
 JOURNAL: Journal
 LANGUAGE: English
 AB QSAR studies were carried out on a few non-benzodiazepine series of compounds, such as 3-substituted-indazole(1,2-b)pyridazines, 2-phenylindazole(1,2-b)pyridazines, 2-(alkoxyphenyl)indazole(1,2-b)benzothiazoles, and 2-aryloquinolines. For the first series of compounds, a

a Fujita-Kan approach was followed, which revealed the highest activity contribution for 3,4-OCD group of 2-Ph moiety and for a methoxy group at 6-position. For the rest of the series, a Ransch approach has been adopted. The hydrophobic and electronic properties of the various substituents had major roles in the binding of these compounds with the receptor. Based on these studies, a hypothetical model for the drug-receptor interaction has been proposed.

IT 179990-56-2 226412-52-2
 RU RAC (Biological activity or effector, except adverse); RSH (Biological study, unclassified); PEP (Properties); REOL (Biological study) (QSAR of nonbenzodiazepine indazole-benzocyclopyridines and quinolines acting at benzodiazepine receptor)
 RU 179990-56-2 CAPLOS
 CH Benzole acid, 2-[(2-phenyl-4-quinolinyl)oxy]-, ethyl ester (CA INDEX NAME)

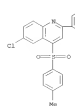


L4 ANSWER 13 OF 25 CAPLOS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1999:160496 CAPLOS
 158143587
 TITLE: Silica-mediated direct condensation of nitroarenes with cinchonyl-type sulfones to yield 2-aryl-4-arylsulfonamides and their hetero analogs
 AUTHOR(S): Wroble, Jolanta
 CORPORATE SOURCE: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, PL-01-224, Pol.
 SOURCE: Tetrahedron (1999), 55(11), 2607-2618
 PUBLINE: COORDINATE NUMBER: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 JOURNAL: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 128:24967
 AB HET/Alkene mediated double condensation of nitroarenes with cinchonyl-type sulfones proceeds smoothly to yield 2-aryl-4-arylsulfonamides and their hetero analogs. Artylsulfonamides can be easily replaced by different nucleophiles.
 IT 204913-37-1F 204913-34-8F 204913-36-8F
 204913-37-1F 204913-38-2F 204913-39-2F
 204913-40-6F 204913-41-7F 204913-42-8F
 RU SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RU 204913-37-1 CAPLOS
 CH Quinoline, 2-phenyl-4-(phenylsulfonamido)- (CA INDEX NAME)



RU 204913-34-8 CAPLOS
 CH Quinoline, 4-chloro-2-(4-(chlorophenyl)-4-[(4-methylphenyl)sulfonyl]- (CA INDEX NAME)



04/17/2008

10-598,246.trn

L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 RI 204913-36-0 CAPLUS
 CH Quinoline, 7-chloro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



RI 204913-37-1 CAPLUS
 CH Quinoline, 6-bromo-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



RI 204913-38-2 CAPLUS
 CH Quinoline, 6-chloro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



RI 204913-39-3 CAPLUS
 CH Quinoline, 6-(methylsulfonyl)-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)

L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 IT 204913-37-1p 204913-35-3p
 RI: NCT (Reactant); STN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 [preparation of (aryl)quinolines via silane-mediated condensation of haloarenes with oxime-type sulfones]
 RI 204913-37-7 CAPLUS
 CH Quinoline, 6-chloro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



RI 204913-35-3 CAPLUS
 CH Quinoline, 6-chloro-4-[(4-methylphenyl)sulfonyl]-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD

L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 204913-40-6 CAPLUS
 CH Quinoline, 2-phenyl-4-(phenylsulfonyl)-6-(trifluoromethyl)- (CA INDEX NAME)



RI 204913-41-7 CAPLUS
 CH Quinoline, 2-phenyl-4-(phenylsulfonyl)-7-(trifluoromethyl)- (CA INDEX NAME)



RI 204913-42-8 CAPLUS
 CH Quinoline, 6-methoxy-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 159410390 CAPLUS
 DOCUMENT NUMBER: 155104154
 TITLE: Oxidations as biotransformations of aromatic functionalities. 15
 AUTHOR(S): Andersen, K. E.; Lundt, B. F.; Joergensen, A. S.; Braastad, C.
 CORPORATE SOURCE: Novo Nordisk A/S, Maaloev, 2760, Den.
 SOURCE: European Journal of Medicinal Chemistry (1996), 31(5), 417-428
 CODEN: EJMCA5; ISSN: 0223-5224
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CONSTRUCT 155104154

AB To improve the in vivo efficacy of a series of known benzodiazepine receptor (R1) ligands, 1-(2-phenyl-4-quinolyl)-4-piperidinecarboxamides, a series of analogs has been prepared in which the amide group of these ligands has been replaced by a 1,1,1-trifluoroethyl moiety or converted to other esterifiable functions such as esters or nitriles. An increase in the in vivo efficacy was observed for some of the compounds prepared in this investigation compared to the parent carboxamide derivative.

IT 178990-56-22
 RI: RAC (Biological activity or effector, except adverse); B5U (Biological study, unclassified); PREP (Preparation); NCT (Reactant); STN (Synthetic preparation); THF (Therapeutic use); R1OL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 [Preparation of 1-(2-phenyl-4-quinolyl)-4-piperidinecarboxamides analogs as benzodiazepine receptor ligands]
 RI 178990-56-2 CAPLUS
 CH Benzoic acid, 2-[1-(2-phenyl-4-quinolyl)oxy]-, ethyl ester (CA INDEX NAME)



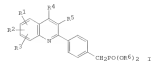
IT 178990-57-3p
 RI: RAC (Biological activity or effector, except adverse); B5U (Biological study, unclassified); PREP (Preparation); STN (Synthetic preparation); THF (Therapeutic use); R1OL (Biological study); PREP (Preparation); USES (Uses)
 [Preparation of 1-(2-phenyl-4-quinolyl)-4-piperidinecarboxamides analogs]

14 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
as histidine/threonine receptor ligands)
AB 178995-51-3 CAPLUS
CD Benzamide, N-ethyl-3-[(2-phenyl-4-quinolinyl)oxyl]- (CA INDEX NAME)



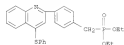
14 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993-495460 CAPLUS
DOCUMENT NUMBER: 119-95360
TITLE: Preparation of quinolines as hypoglycemic and antidiabetic
INVENTOR(S): Muta, Kazuyuki; Shoji, Yasuo; Tada, Yoshiko; Tsutsumi, Kazuhiko; Kamisaka, Kiji; Inoue, Yasuhiko
SOURCE: Otsuka Pharma Co Ltd, Japan
PATENT ASSIGNMENT(S): Jpn. Kokai Tokkyo Koho, 11 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 0504359	A	1993-02-23	JP 1992-13186	1993-01-10
PRIORITY APPL. INFO.			JP 1991-102184	A1 1991-02-05
OTHER SOURCE(S):			NAFAT 119-95360	
CI				



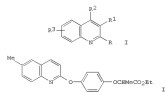
AB The title compd. 1 [R1-R3 = H, lower alkyl, lower alkoxy, halo, NO2; R4, R5 = H, lower alkyl, (halo-substituted) Ph, Ph, CH₃, cyano, lower alkoxy, lower alkoxy, halo; R6 = lower alkyl], useful as hypoglycemic and antidiabetic (no data), are prepared including 2-(4-g-tolyl-4-methylphenyl)-4-phenylquinoline with R6 and R5(O). In C586 for 15 h gave 24.0 g 2-(4-bromomethylphenyl)-6-chloro-4-phenylquinoline, which (10.3 g) was treated with tri-ethyl phosphite at 160°C for 1 h to afford 7.2 g 1 [R1 = 6-Cl, R2 = R3 = R5 = H, R4 = Ph, R6 = Et].
IT 149135-10-22
RI: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as hypoglycemic and antidiabetic agent)
IN 149135-10-2 CAPLUS
CN Phosphonic acid, [[4-[4-(phenylthio)-2-quinolinyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

14 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



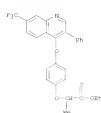
14 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992-098123 CAPLUS
DOCUMENT NUMBER: 97-198123
ORIGINAL REFERENCE NO.: 97-33191A, 33184A
TITLE: Quinolines/phenylpropanoic acid derivatives and their use as herbicides
INVENTOR(S): Milkenberger, Rainer; Boer, Harald; Bauer, Klaus
PATENT ASSIGNMENT(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 20 pp.
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3102144	A1	1980-09-18	DE 1981-3101544	1991-01-10
PRIORITY APPL. INFO.				
OTHER SOURCE(S):			CASREACT 97-198123	
CI				

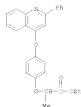


AB I [one of R1 or R2, especially R = 4-ROCH2CO2Et or CO2H or a derivative, e.g. amide] and the other = H, Cl-4 alkyl, Ph, Cl, Br, R1 = H, Cl-4 alkyl, Cl, Br, cyano, Cl-4 esteralkoxy; R3 = H, Cl-4 alkyl, alkoxy, or dialkylamino, NO2, CF3, halo; n = 0-3] were prepared as herbicides. Thus, 21 g 4-ROCH2CO2Et were added dropwise to 2.9 g NaH in 100 mL DMS, 17.7 g 2-chloro-4-methylquinoline added, and the mixture was stirred 2 h at 100°C to give 89.28 g II.
IT 87556-48-29 STN-71-89
RI: AGS (Agricultural use); BAC (Biological activity or effector, except adverse); B01 (Biological study, unclassified); SPN (Synthetic preparation); BTOL (Biological study); PREP (Preparation); USEP (Use)
(preparation of, as herbicide)
IN 87556-48-3 CAPLUS
CN Propanoic acid, 2-[4-[3-phenyl-7-(trifluoromethyl)-4-quinolinyl]oxy]phenyl-, ethyl ester (CA INDEX NAME)

14 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RI 53596-71-8 CAPLUS
 CH Propanoic acid, 2-[(4-{[2-phenyl-4-quinolinyl]oxy}phenyl)-ethyl ester
 (CA INDEX NAME)



14 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



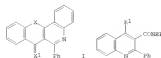
RI 65031-30-3 CAPLUS
 CH 3-Quinolincarboxamide, 2-phenyl-4-(phenylthio)- (CA INDEX NAME)



RI 65031-32-5 CAPLUS
 CH 3-Quinolincarboxamide, N,2-diphenyl-4-(phenylthio)- (CA INDEX NAME)



14 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1978:22706 CAPLUS
 DOCUMENT NUMBER: 88122706
 ORIGINAL REFERENCE NO.: 8812454,3648a
 TITLE: Synthesis and structure of some new heterocyclic analogs of benzanthracene
 AUTHOR(S): Naka, Marian
 CORPORATE SOURCE: Inst. Chem., Jagiellonian Univ., Krakow, Pol.
 SOURCE: Mazuryi Nieszkowe Uniwersytetu Jagiellońskiego, Prace Chemiczne (1978), 21, 171-7
 CODEN: IJACPAJ ISSN: 0373-0146
 DOCUMENT TYPE: Journal
 LANGUAGE: English

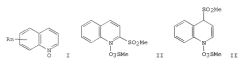


AB Condensed quinolines I (R = O, S, N, R1 = O) were obtained by treating II (R = R1 = Cl) with PhNH2 and cyclizing II (R = R1 = Cl) with polyphosphoric acid. Treatment of II (R = Ph, R1 = Cl) with PhNH2 and cyclization of II (R = Ph, R1 = NH2) gave I (R = O, R1 = NH2), which were hydrolyzed to I (R1 = O).
 IT 65031-36-7F 65031-38-3F 65031-30-3P
 65031-32-5P
 RI: RCT (Reactant); RSM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 CH (Preparation and cyclization of)
 RI 65031-36-7 CAPLUS
 CH 3-Quinolincarboxamide, 4-phenoxy-2-phenyl- (CA INDEX NAME)



RI 65031-28-9 CAPLUS
 CH 3-Quinolincarboxamide, 4-phenoxy-2-phenyl- (CA INDEX NAME)

14 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1977:16744 CAPLUS
 DOCUMENT NUMBER: 87167446
 ORIGINAL REFERENCE NO.: 8716511a,16512a
 TITLE: The reaction of heteroaromatic N-oxide with acid chloride and cyanide. The reaction of quinoline N-oxide with sulfonic acid chloride and potassium cyanide
 AUTHOR(S): Miyachi, Etsuro; Shimada, Noriaki
 CORPORATE SOURCE: Shirooka Coll. Pharm., Shirooka, Japan
 SOURCE: Yakugaku Zasshi (1977), 97(8), 627-60
 CODEN: YAKUJZ ISSN: 0014-9991
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese



AB Reaction of 17 quinoline oxides I (e.g., R = H, Me, NO2, Ph, CH3, halo) with CCl4 and KCN gave the 2-(methylsulfonyl)quinolines or, when the 2-position was substituted, the 4-(methylsulfonyl) derivs. via elimination of SO2Me from the intermediates II or III.
 IT 64495-42-1F 64495-43-1P
 RI: PREP (Preparation)

(By reaction of quinoline oxide derivative with sulfonic acid chloride)
 RI 64495-42-1 CAPLUS
 CH Quinolines, 2-(4-methylphenyl)-4-(phenylsulfonyl)- (CA INDEX NAME)



RI 64495-43-2 CAPLUS
 CH Quinolines, 2-(4-methylphenyl)-4-(phenylsulfonyl)- (CA INDEX NAME)

14 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN (Continued)



NO 30413-12-8 CAPLUS
 CH 3-Quinolinecarboxylic acid, 5-methyl-2-(2-nitrophenyl)-4-phenoxy-, ethyl ester (8C1) (CA INDEX NAME)



NO 30413-13-9 CAPLUS
 CH 3-Quinolinecarboxylic acid, 7-methyl-2-(2-nitrophenyl)-4-phenoxy-, ethyl ester (8C1) (CA INDEX NAME)



14 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 1971:53602 CAPLUS
 DOCUMENT NUMBER: 74:53602
 ORIGINAL REFERENCE NO.: 74:5374, 5604a
 TITLE: Cyclic amides. XIII. 1,6-dimethyl-2-(2-nitrophenyl)-4-phenoxy-2,3,4-de[1,6]naphthyridines and their molecular orientation
 AUTHOR(S): IN CARCINOGENESIS
 Katrik, Maurice M.; Bloomfield, R. G.; Vipond, H. J.
 CORPORATE SOURCE: Univ. Nottingham, Nottingham, UK
 SOURCE: Journal of the Chemical Society (Section C): Organic (1970), 119, 2841-53
 CURRENT COUNTRY: IRELAND 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 CI: For diagram(s), see printed CA issue.
 AS: Cyclizations of substituted diene[5,6,11,12]naphthyridines and of substituted [1]benzopyran[7,2-c]quinolin-7-one, and the condensation of N-carboxanthranilic acid anhydrides with substituted 1,3-diphenylpropene 1,3-diones followed by a reductive cyclization, leading unequivocally to diene[5,6,11]benzopyran[7,2-c]quinolin-7-one, and five isomeric Me derive, are described. An explanation is given of the difference in carcinogenic activity of the 2-, 7-, and 12-methyl derive, consistent with specific mol. orientations for carcinogenesis similar to those deduced for triepoxyquinoline and its derive.
 IT 30413-10-69 30413-11-70 30413-12-80
 30413-13-90
 RU: SYN (Synthetic preparation); PREP (Preparation) (preparation of)
 RU 30413-10-6 CAPLUS
 CH 3-Quinolinecarboxylic acid, 2-(2-nitrophenyl)-4-phenoxy-, ethyl ester (8C1) (CA INDEX NAME)



RU 30413-11-7 CAPLUS
 CH 3-Quinolinecarboxylic acid, 2-(2-nitrophenyl)-4-phenoxy-, ethyl ester (8C1) (CA INDEX NAME)

14 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 1958:25581 CAPLUS
 DOCUMENT NUMBER: 52:25581
 ORIGINAL REFERENCE NO.: 52:4658C-1, 4658A-1
 TITLE: Triazaphenanthrenes. II. Derivatives of 10-phenyl-1,2,3-triazaphenanthrene
 Aikawa, G. M.; Matsuda, A. R.
 SOURCE: Journal of the Chemical Society (1957) 2722-6
 CURRENT COUNTRY: IRELAND 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CSEARCH 52:25581
 AS: A preparative route to 4-acetyl-3-amino-2-phenylquinoline (I) was developed. Purification of I in HCl and subsequent cyclization gave chiefly 4-acetyl-3-chloro-2-phenylquinoline (II), with 10% of the hydroxytriazaphenanthrene (III) or 60% yield of III was obtained by cyclization in an alkaline medium.
 4-Amino-10-phenyl-1,2,3-triazaphenanthrene (IV) formed a mesomerically inactive 2-phenyl-3-phthalimidoquinoline-4-carboxylic acid (VI) (40 g.) refluxed 0.5 hr. with 400 cc. 50% volume/volume H2SO4 gave
 3-amino-2-phenylquinoline (VII), m. 113°. Neutralization of the mother liquors and rearin. with HCl gave 3-amino-2-phenylquinoline-4-carboxylic acid (VIII), m. 254°. VI was recovered after 2 hrs. heating with 30% on 75% NaOH. VII was also formed by similar treatment of 2-phenyl-2-phthalimidoquinoline (IX). VI (2.5 g.) and 15 cc. H2SO4 heated 1 hr. at 215° gave IV, m. 249-50° (C86). The presence of VII in the aqueous mother liquors was indicated by its fluorescence and by the sublimate of phthalic anhydride in the condenser. VII (18 g.) in 45 cc. H2O and 75 cc. concentrated HCl dissolved at 0° with 5 g. NaOH, the solution treated at 0° in 54 g. SnCl2 and 54 cc. concentrated HCl and 100 cc. H2O, the mixture kept 0.5 hr. at 0°, allowed to come to room temperature overnight, diluted to 1500 cc., partially neutralized with 25 g. NaOH in 50 cc. H2O, the Sn salt removed as the sulfide, and the precipitate collected, then digested with refluxing H2O, the combined filtrates concentrated to 350 cc. and then cooled gave 3-hyazano-2-phenylquinoline-HCl(I), m. 255° (decomposition). The hydrazones of H2Me (XI) (16 cc.) prepared from 10 g. of 3 by refluxing 5 min. with 16 g. MeOH in 16 cc. H2O and 25 cc. alc. in 9.3 g. yield, m. 123° aqueous alc.). The derivative (XIIa) from PhOAc, prepared by the same method, was a sticky solid which could not be crystallized XI (9.3 g.) heated 6 hrs. with 80 cc. concentrated HCl gave 5.9 g. 4',5'-dimethyl-2-phenylpyrrolo-[2',3'-5,4]quinoline (XII) HCl, m. about 305° (variable). XII HCl from alkaline with HCl gave free XII, needles, m. 304-5° (C86). XII was recovered unchanged after 4.5 hrs. heating with either AcCl or Ac2O. Crude XIIa (2.2 g.) heated 6 hrs. with 50 cc. concentrated HCl gave
 4'-methyl-2,5'-diphenylpyrrolo-[2',3'-5,4]quinoline-HCl, m. about 305° (variable). VI (10 g.) refluxed 0.5 hr. with 30 cc. SnCl2 and then heated 0.5 hr. with 50 cc. alc. gave II. 2-phenyl-3-phthalimidoquinoline-4-carboxylate, leaflets, m. 192-3°

14 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 mol. PMSE gave 5.98 V, 0.02 mol. 1 and 0.04 mol. PMSE gave 5.9 V, 0.28 IV,
 and 1.7 g. (PMSE)2CO. The PMSE/PCPDCB (from 3.8 g. 1 and 1.7 g.
 PMSE), cyclized in 25 on 60 sec. PMSE, gives 4.7 and 3.8 V, resp.
 IT 856719-92-2P, Quinoline, 6-chloro-4-phenoxy-3-phenyl-
 RU: PREP (Preparation)
 (preparation of)
 RU 856719-92-2 CAPLUS
 CN Quinoline, 6-chloro-4-phenoxy-3-phenyl- (CA INDEX NAME)



14 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1928:20202 CAPLUS
 DOCUMENT NUMBER: 22120202
 ORIGINAL REFERENCE NO.: 22125553-1
 TITLE: Quinoline derivatives. VIII. Compounds of
 2-phenyl-4-hydroxyquinoline
 AUTHOR(S): John, Hans; Wunscher, K
 SOURCE: Journal fuer Praktische Chemie (Leipzig) (1926), 119,
 42-8
 CUBIN: JPCSAQ ISSN: 0021-8383
 DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
 AB str. C. A. 22, 426. 2-Phenyl-4-acetoxyquinoline, m. 70°; picrate.
 EtO derivative, m. 90-17°; picrate, 4-EtO derivative, m. 100-2°;
 various salts of this and the following are described. 4-370
 derivative, pale
 yellow, m. 252°. 4-n-Crotony derivative, m. 241-3°.
 4-p-Nitrophenoxy derivative, m. 88-90°. 4-p-Aminophenoxy derivative, m.
 91°. 4-o-Methoxyphenoxy derivative, m. 246°. 4-o-Isopropoxy-
 n-methoxyphenoxy derivative, m. 252°. All but the last two
 deriva. were prepared from the 4-Cl derivative
 IT 856837-34-2P, Quinoline, 4-(p-aminophenoxy)-3-phenyl-
 856888-26-2P, Quinoline, 2-phenyl-4-n-toloxyl-856888-31-8P
 , Quinoline, 4-(p-nitrophenoxy)-2-phenyl- 856896-43-6P,
 Quinoline, 4-(2-isopropyl-5-methoxyphenoxy)-2-phenyl- 856896-70-3P
 , Quinoline, 4-phenoxy-2-phenyl- 856896-72-3P, Quinoline,
 6-(o-methoxyphenoxy)-2-phenyl-
 RU: PREP (Preparation)

(preparation of)
 RU 856837-34-2 CAPLUS
 CN Quinoline, 4-(p-aminophenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



RU 856888-26-1 CAPLUS
 CN Quinoline, 2-phenyl-4-n-toloxyl- (3C1) (CA INDEX NAME)

14 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RU 856888-31-8 CAPLUS
 CN Quinoline, 4-(p-methoxyphenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



RU 856896-43-6 CAPLUS
 CN Quinoline, 4-(2-isopropyl-5-methoxyphenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



RU 856896-70-3 CAPLUS
 CN Quinoline, 4-phenoxy-2-phenyl- (CA INDEX NAME)

14 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RU 856896-72-3 CAPLUS
 CN Quinoline, 4-(o-methoxyphenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



04/17/2008

10-598,246.trn

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SESSION

FULL ESTIMATED COST

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319.60

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SINCE FILE

ENTRY

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SESSION

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